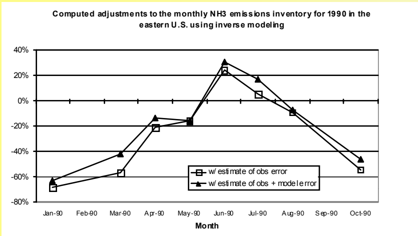
Advances in Emissions Modeling of Airborne Substances

Thomas Pierce*, William Benjey*, Jason Ching*, Dale Gillette*,
Alice Gilliland*, Shan He+, Michelle Mebust, and George Pouliot*
Atmospheric Modeling Division
National Exposure Research Laboratory
U.S. Environmental Protection Agency
Research Triangle Park, NC

Objective: In support of air quality modeling, the Atmospheric Modeling Division is seeking to improve emission estimates by building emission models that account for meteorological conditions and by developing innovative ways for evaluating emission inventories.

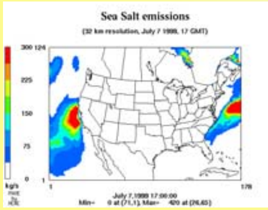
Inverse Modeling to Estimate Seasonal Ammonia Emissions

➢ The magnitude and temporal variability of ammonia (NH_3) emissions is highly uncertain. Distributing NH_3 emissions evenly over the year can adversely affect air quality model-predicted concentrations of nitrogen-containing compounds.
➢ Inverse modeling optimizes modeled concentrations by modulating emission inputs.
➢ We have used this approach to estimate seasonally-varying NH_3 emissions, based on the Community Multiscale Air Quality (CMAQ) model and ammonium wet concentration observations from the National Atmospheric Deposition Program.
➢ Inverse modeling produced strong seasonal differences in NH_3 emissions; NH_3 emissions are more than 75% lower during the winter than the summer. More details can be found in Gilliland *et al*. (*Journal of Geophysical Research*, in press).



Sea Salt Emissions

➢ The aerosol module within the CMAQ modeling system needs to account for sea salt emissions over marine environments.
➢ Among available sea spray generation functions, Smith and Harrison (*Journal of Aerosol Science* **29**:S189-S190, 1998) appear best-suited for CMAQ.
➢ Their equations have been adapted to compute sea salt emissions as a function of marine area, vertical wind profile, and roughness length.
➢ A test case using a version of CMAQ has been created with a 32-km gridded national domain for a 15-day period in July 1999.
➢ Analysis of the gridded emission estimates and CMAQ simulations is planned.



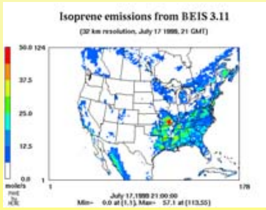
Support for the Sparse Matrix Operational Kernel Emissions System

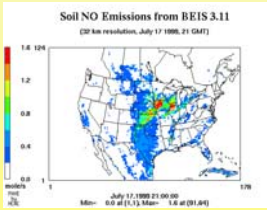
➢**Background:** SMOKE began under the sponsorship of the Atmospheric Modeling Division with the North Carolina Supercomputing Center. As a community model, it is applicable to any pollutant, computationally efficient, and architecturally flexible. SMOKE may be downloaded at www.cmascenter.org.
➢**Recent enhancements:**
- Group major elevated point sources by stack parameters, emissions, plant ID, source ID, and plume rise (Benjey et al., *Proceedings of the 10th Emission Inventory Conference*, 2001).
- Specify source category and geographically-specific factors for controls, future projections, adjustments, and reactivity analyses.
- Speciate for the CB4, RADM2, or SAPRC chemical mechanisms.

In collaboration with EPA's OAQPS, SMOKE will provide toxic emissions for CMAQ. The initial implementation of toxic emissions in SMOKE is limited to the Carbon Bond 4 mechanism and mobile sources, but other source types will soon follow.
➢**Spatial allocation:** Gridding spatial data poses a difficult challenge when processing raw emissions data. A new program, Spatial Allocator, has replaced SMOKE Tool that was part of the old Models-3 modeling framework. Unlike SMOKE Tool, Spatial Allocator does not require the use of expensive proprietary software. Downloads are available at www.epa.gov/AMD/mims/software/spatial_allocator.html.

Biogenic Emissions Modeling

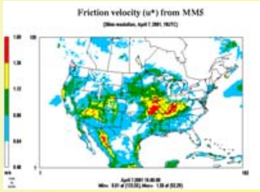
➢**Biogenic Emissions Inventory System (BEIS)** was introduced in 1988 to estimate VOC emissions from vegetation and NO emissions from soils.
➢**BEIS3.09** is the default version in SMOKE (Vukovich and Pierce, 2002, www.epa.gov/ttn/chief/conference/ei11/modeling/vukovich.pdf).
➢**BEIS3.10** is a research version for CMAQ. It includes a 1-km vegetation database that resolves forest canopy coverage by tree species; emission factors for 34 chemicals, including 14 monoterpenes and methanol; a soil NO algorithm dependent on soil moisture, crop canopy coverage, and fertilizer application; and, speciation for the CBIV, RADM2, and SAPRAC99 mechanisms (Pierce et al., 2002, ams.confex.com/ams/AFMAPUE/12AirPoll/abstracts/37962.htm).
➢**BEIS3.11** revises the soil NO algorithm in BEIS3.10 to better distinguish between agricultural and non-agricultural land, and to limit adjustments from temperature, precipitation, fertilizer application, and crop canopy to the growing season and to areas of agriculture. A leaf shading algorithm is added for estimating methanol emissions from non-forested areas. BEIS3.11 is available for testing at www.epa.gov/asmdnerl/biogen.html.

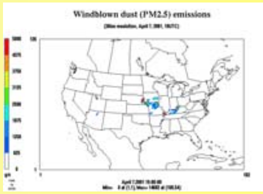




Fugitive Dust Emissions

➢ Fugitive dust emissions tend to be overestimated in atmospheric transport models (Gillette, 2001, www.wrapair.org/forums/dejf/documents/FugativeDustFinal.doc)
➢To account for this discrepancy, He et al. (2002, Proceedings of the Annual Conference of the American Association for Aerosol Research, Charlotte, NC) developed an algorithm for CMAQ based on the work of Gillette.
➢ The algorithm uses threshold friction velocity parameterizations and incorporates gridded databases of soil type, surface soil moisture content, weather, and vegetation.
➢ The algorithm also tries to account for the sub-grid scale variability caused by the non-homogeneities in the distribution of land use, and the interception of the uplifted dust particles by vegetation.
➢CMAQ simulations have begun and are being evaluated for a multi-day windblown dust episode that occurred during April 2001.
➢ We plan to implement the algorithm into CMAQ by 2004.





Wildland Fire Emissions

➢We are collaborating with the National Park Service and the Cooperative Institute for Research in the Atmosphere to develop a stand-alone processor for simulating emissions from wildland fires.
➢Our goal is to build a national tool with the following characteristics: (1) horizontal resolutions from 1 to 36 km; (2) temporal resolution from hourly to multi-year; and, (3) chemical speciation for criteria pollutants and their precursors.
➢The Community Smoke Emission Model (CSEM) is a prototype consisting of algorithms developed primarily by the US Forest Service (USFS).
➢Initial results from the CSEM prototype have been presented by Sestak et al. (www.cmascenter.org/workshop/session5/fox_abstract.pdf, 2002).
➢Plans are being made to evaluate CSEM with the fire emissions from the Western Regional Air Partners' (WRAP) Fire Emissions Forum. The USFS plans to integrate CSEM into SMOKE and CMAQ and to distribute CSEM via the CMAS website.

Contact: Thomas Pierce (Email: pierce.tom@epa.gov)

*On assignment from Air Resources Laboratory, National Oceanic and Atmospheric Administration.

+On assignment from the University Center for Atmospheric Research.